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Drake
5355
Hawkins

AFOSR Molecular Dynamics and Theoretical Chemistry Contractors Meeting (Statement A)
(San Diego, CA, 18-20 May 2003) (Deadline: 14 Apr 2003)

Structural Effects on the Physical Properties of Ionic Liquids

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Recently work using ionic liquids has risen exponentially in both academic research efforts as well as by industrial large-scale organic synthesis. Much of these efforts have centered around the use of di-alkyl substituted imidazolium salts with an array of anions, many of which are commercially available. The pioneering work carried out by the USAF in the last several decades has shed some light upon some of the physical property effect relationships of increasing the alkyl side chain length of these imidazolium cations with viscosities, melting points, hygroscopicity/hydrophobicity, and densities. However, most researchers in the field today are forging efforts in using ionic liquids in various aspects of synthesis and separations, as part of the environmentally driven "green chemistry" efforts. In our efforts we are coming to terms with what really drives the physical properties of ionic liquids and how we are beginning to understand the cation anion interactions. Discussions will focus on factors including size and shape of both the cation and anion, hydrogen bonding, charge delocalization on either/both cation and/or anion, in our quest to design, synthesize and charcterize new ionic liquids of interest.